

Molecular Electronics: Charge Transport in Molecular Thin Films on Oxide and Metallic Surfaces

The NIST research described here focuses on experimental and theoretical investigations of the structure and charge transport characteristics of thin films of organic pi systems chemically bound to oxide and metallic surfaces. The structure and molecular organization within the films has a large impact on the through film charge transport. This project supports the broader molecular and organic electronics efforts at NIST.

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Vapor deposition is commonly used to form multilayers of organics that can serve as active elements in device structures. The molecular structure within these as-deposited films is closely related to the bulk crystal structure of the molecules. This bulk crystal structure usually consists of a herringbone type arrangement of the molecules, which has been shown, theoretically, to have a large impact on the charge transport in organic and molecular based devices. New methods for solution phase deposition and optimization of charge transport of active organic/molecular layers is of interest for more efficient devices.

In the NIST approach, solution phase chemical methods are used to tether the active molecules to the surface to form ordered monolayer films of charge transport moieties. Our initial theoretical simulations of these types of structures reveal their potential as active layers in monolayer organic devices.

These studies predict that better molecular overlap can be achieved by chemically binding the pi systems to the surface via an alkyl chain (Figure 1). By anchoring the molecules to the surface, the herringbone structure of the bulk crystals is not predicted and the calculated charge transport (mobility) within well-ordered films is comparable to that of vapor deposited systems as reported in the literature. Charge mobilities were calculated for each of the nearest-neighbor interactions in the films of pyrene (hole transport agent) and 2,1,3-benzoxadiazole-5-carboxylic acid (electron transport agent) tethered to the

SiO₂ surface. For pyrene (Figure 1), the calculated hole mobilities (A= 12.869 cm²/V·s ; B= 9.299 cm²/V·s; C= 0.138 cm²/V·s) show that the most efficient charge transport in the pyrene film is in the direction of A.

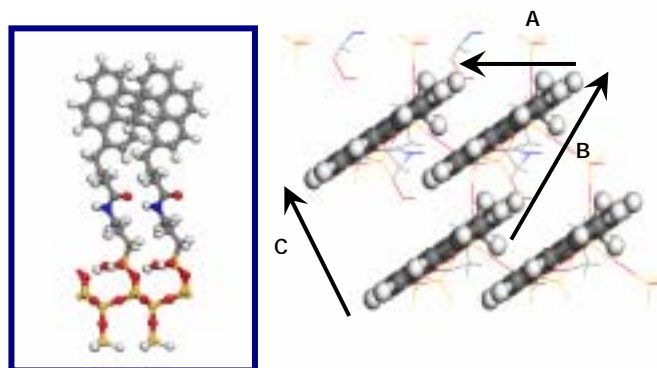


Figure 1. Side-on (left) and top-down view (right) of pyrene film attached to SiO₂ surface via alkyl linker. Hole mobilities were calculated for each nearest neighbor interaction and are listed in text.

While theoretical investigations of these films show their promise for creating efficient devices at the monolayer level, experimental studies show the challenges of making such films a reality. In our studies, a number of bottom-up chemical assembly methods were explored to create monolayers of charge transport agents tethered to the SiO₂ surface (Figure 2 on next page). Film formation was characterized using AFM, FTIR, contact angle and ellipsometric techniques. Following optimization of these attachment techniques, films were incorporated into field effect transistor device structures for analysis of their charge transport characteristics. These devices were created using photolithographic methods and did not show transistor characteristics. We believe that these results are related to two different factors including: (1) the size (channel length and width) of devices made using photolithographic techniques and (2) the irreproducibility of monolayer films of the initial silane linkers.

Future Plans: A combination of FTIR, ellipsometry, contact angle, and STM techniques will be used to determine the influence of alkyl linker chain length on monolayer film formation and order on both Au and SiO₂ surfaces. We will further evaluate what influence ordering within these films may have on solution phase deposition

of additional molecular layers. Theoretical simulations will be expanded to include a variety of charge transport agents tethered to the SiO_2 surface. A comparison of these systems will show the influence of the film structure on the through-film charge transport and will be used as a comparison to the charge transport characteristics of bulk systems presented in the literature.

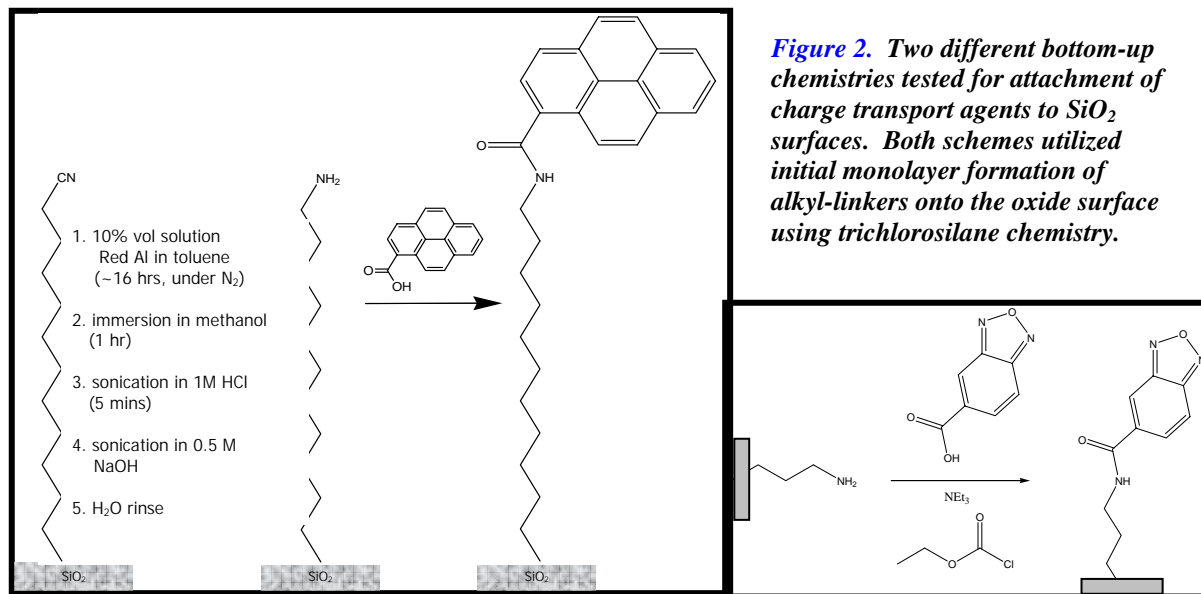


Figure 2. Two different bottom-up chemistries tested for attachment of charge transport agents to SiO_2 surfaces. Both schemes utilized initial monolayer formation of alkyl-linkers onto the oxide surface using trichlorosilane chemistry.